TNSL improvements in FUDGE

CSEWG

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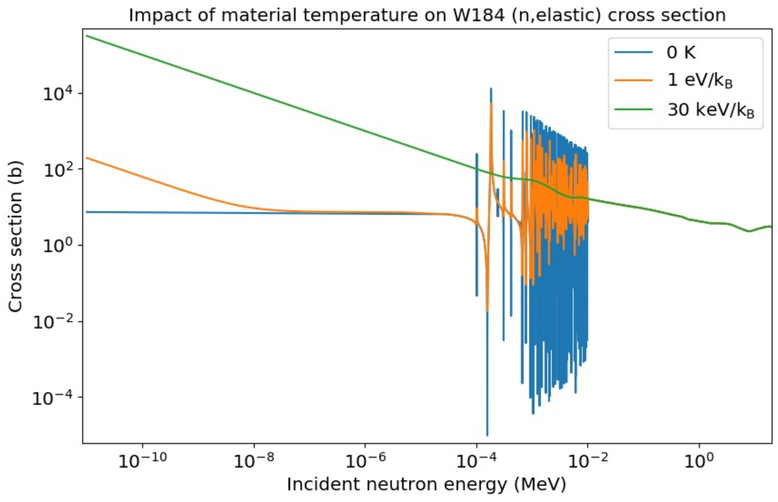
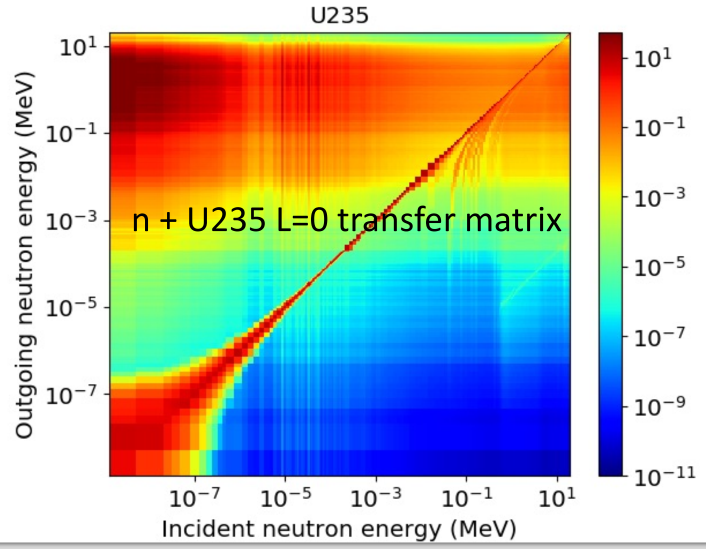
LLNL infrastructure for managing and processing nuclear data

- GNDS: Generalized Nuclear Database Structure
  - New international format for storing evaluated and processed nuclear data
  - Replaces various formats including ENDF-6
- FUDGE: For Updating Data and Generating Evaluations
  - Python based code for modifying, viewing and processing nuclear data
  - Computationally intensive routines written in C and C++
  - FUDGE-5.0 now available at github.com/LLNL/fudge
- GIDI+: General Interaction Data Interface
  - Suite of C++ APIs for accessing GNDS data for use in transport codes
  - Includes API for sampling GNDS data as needed by Monte Carlo codes
  - New release coming soon to github.com/LLNL/gidiplus
- Both codes are open source and used externally





Recent FUDGE development has focused on improving low-energy neutron capabilities, especially for TNSL and URR.

- Thermal Neutron Scattering Law
  - TNSL format specification is changing significantly in GNDS-2.0
  - FUDGE processing implemented, tested various ways
    - Compare directly (processed cross sections and spectra) and indirectly (broomsticks, k_{eff})
    - Some differences for incoherent inelastic require further exploration
  - Now have several methods for getting processed FUDGE results into transport codes
    - GNDS with GIDI+, ACE format, ENDL format with COG library generator or legacy LLNL processing

- Unresolved resonance region
  - FUDGE probability tables (especially for elastic and total) often show narrower cross section range compared to NJOY / FRENDY
  - Working with other code developers to understand that difference

The hierarchy for storing TNSL data was overhauled between GNDS-1.9 and GNDS-2.0

GNDS-1.9

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  +<documentation name="endfDoc"></documentation>
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GNDS-2.0

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...
tic"></outputChannel>
...
 </reactionSuite>
```

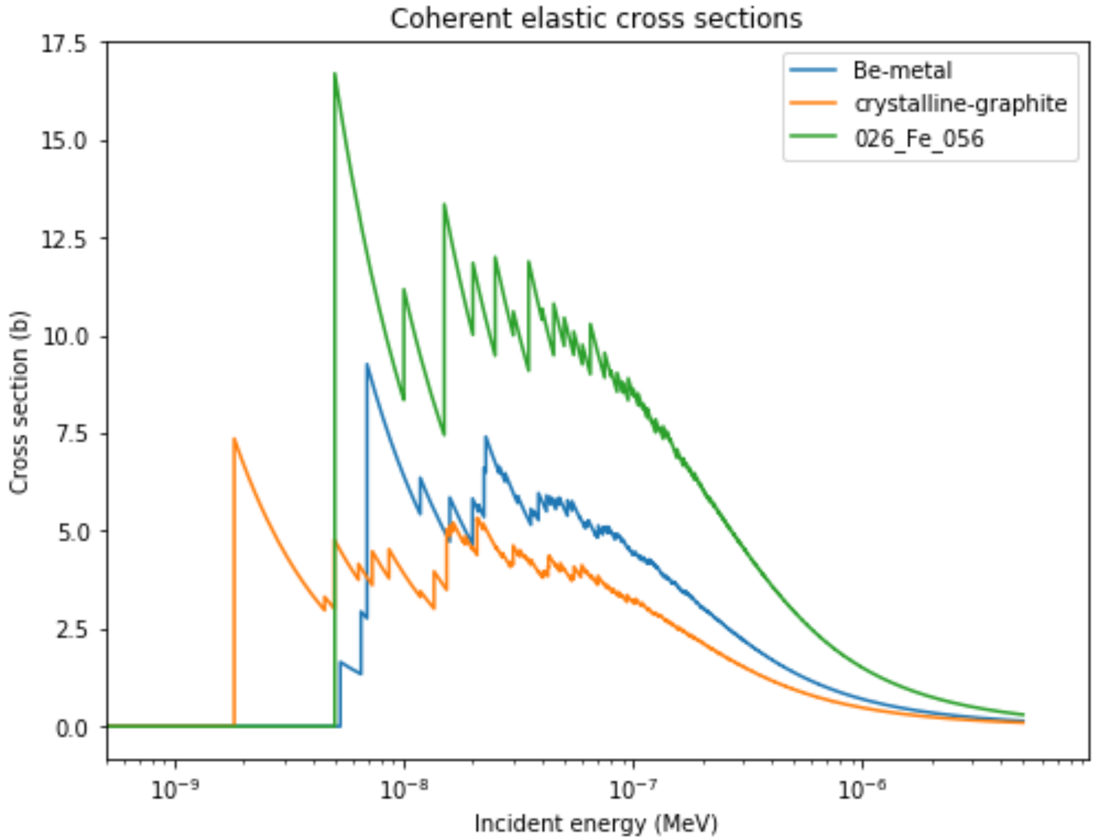
GNDS-2.0 layout integrates TNSL with all other reactions. Integrating and renormalizing TNSL double-differential cross sections produces a standard cross section and outgoing neutron distribution.

Coherent elastic: bulk scattering off crystalline materials

$$\frac{d^2\sigma}{dE'\,d\Omega}(E \rightarrow E', \mu, T) = \frac{1}{E}\sum_{i=1}^{E_i<E} s_i(T)\,\delta(\mu-\mu_i)\,\delta(E-E')/2\pi$$

where

$$\mu_i = 1 - \frac{2E_i}{E}$$

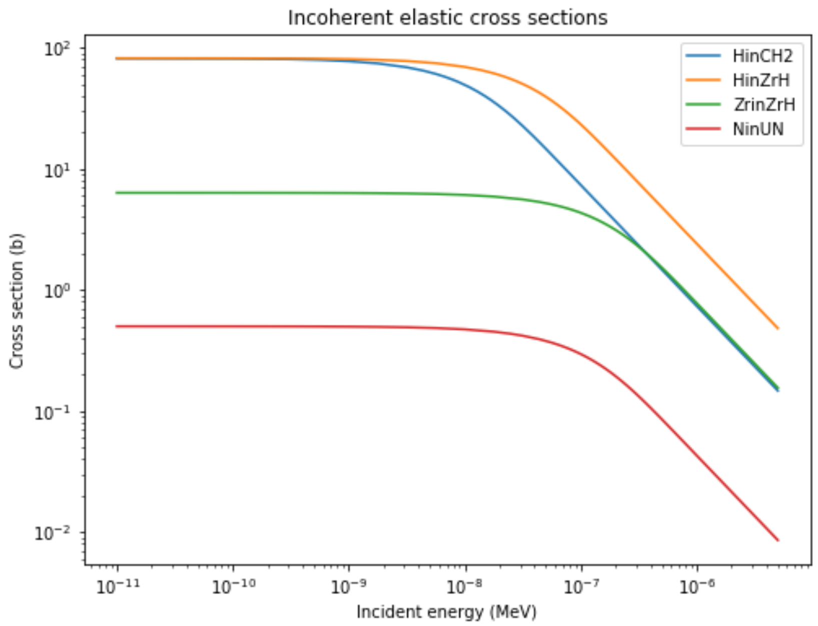


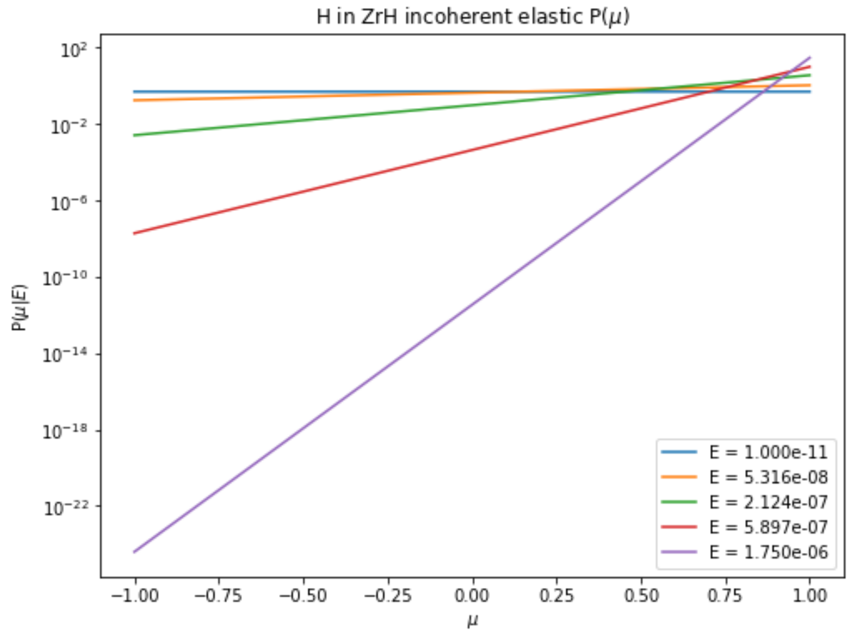
- Outgoing angular distribution consists of delta functions at various μ_i
- TODO: sample angles directly using $s_i(T)$
  - Requires some work in GIDI+

Incoherent elastic: bulk scattering off partially ordered materials

$$\frac{d^2\sigma}{dE'\,d\Omega}(E \to E', \mu, T) = \frac{\sigma_b}{4\pi}\, e^{-2EW'(T)(1-\mu)}\ \delta(E - E')$$

where σ_b and W'(T) are tabulated

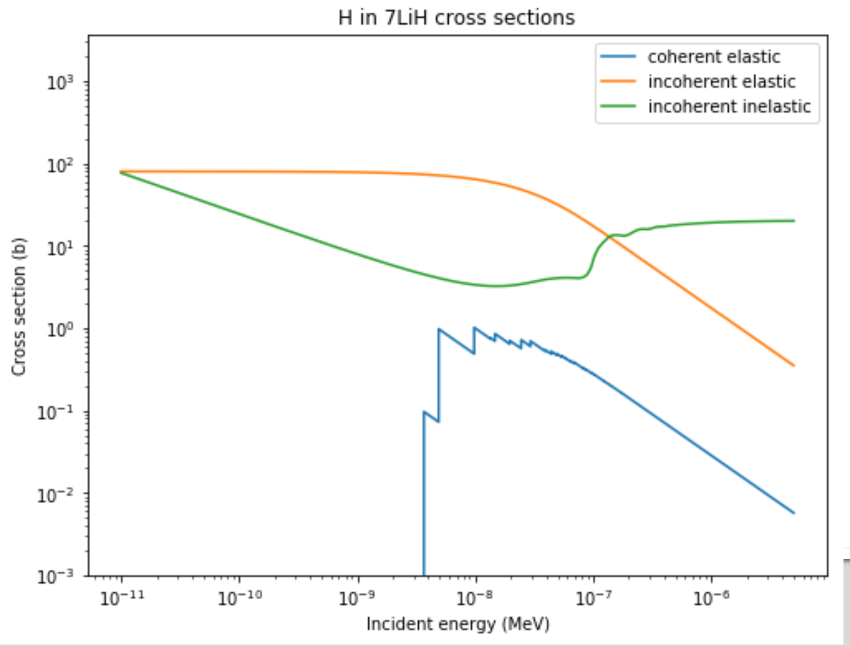


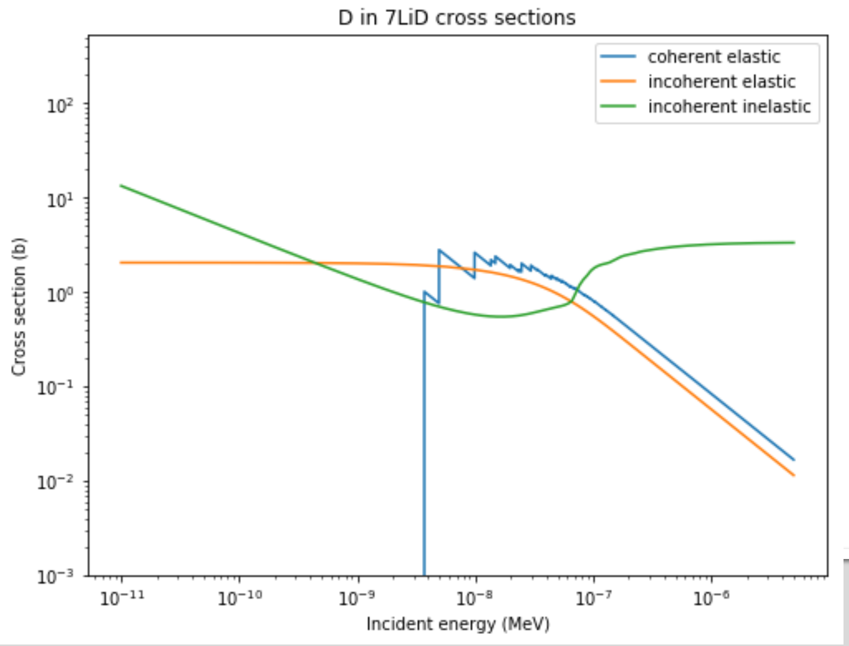


Again, seems more efficient to use W'(T) to sample directly… TBD

GNDS easily handles new LTHR=3 (mixed elastic) format

- Some materials require both coherent elastic and incoherent elastic (plus inelastic) to properly represent thermal scattering region.
- Handled in GNDS simply by adding another ***reaction*** node for the new elastic term
- Example files for ^{7}LiH and ^{7}LiD were translated to GNDS and processed with FUDGE
  - Results can be translated to ENDL, ACE coming soon once we check latest format update…





Incoherent inelastic is trickier, often requires extrapolation beyond tabulated $S_{\alpha\beta}$ grid especially at forward angles.

$$\frac{d^2\sigma}{d\Omega\, dE'}(E \to E', \mu, T) = \sum_{n=0}^{\mathrm{NS}} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S_n(\alpha, \beta, T)$$

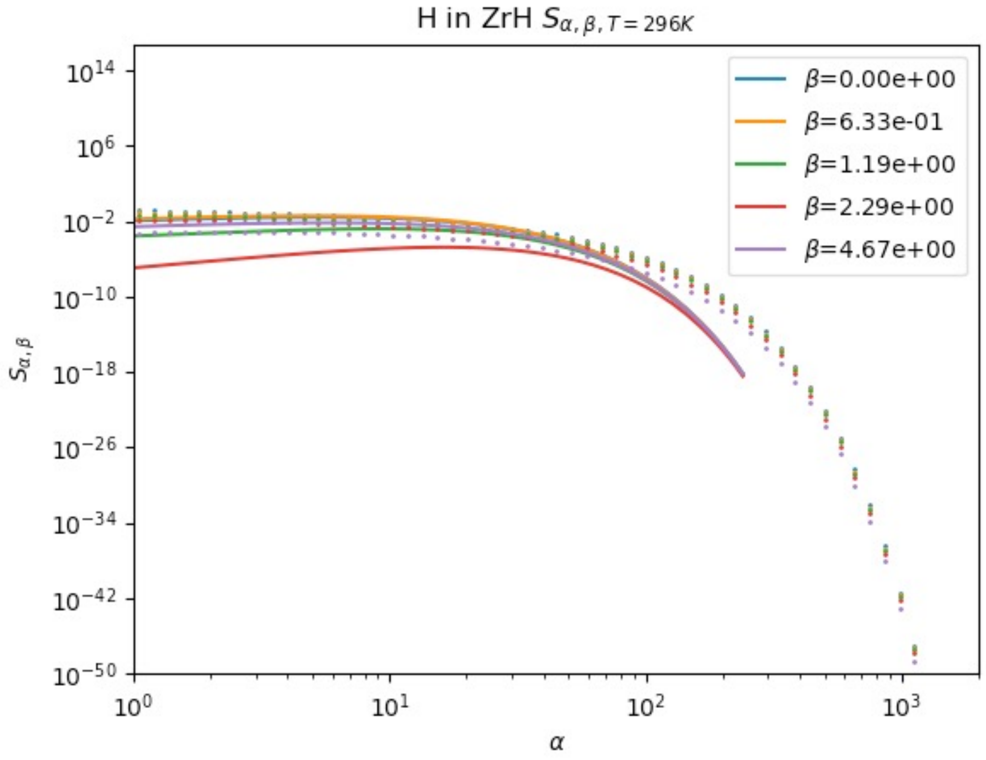
$$\alpha = \left[E' + E - 2\mu\sqrt{EE'} \right] \, /A_0 kT$$

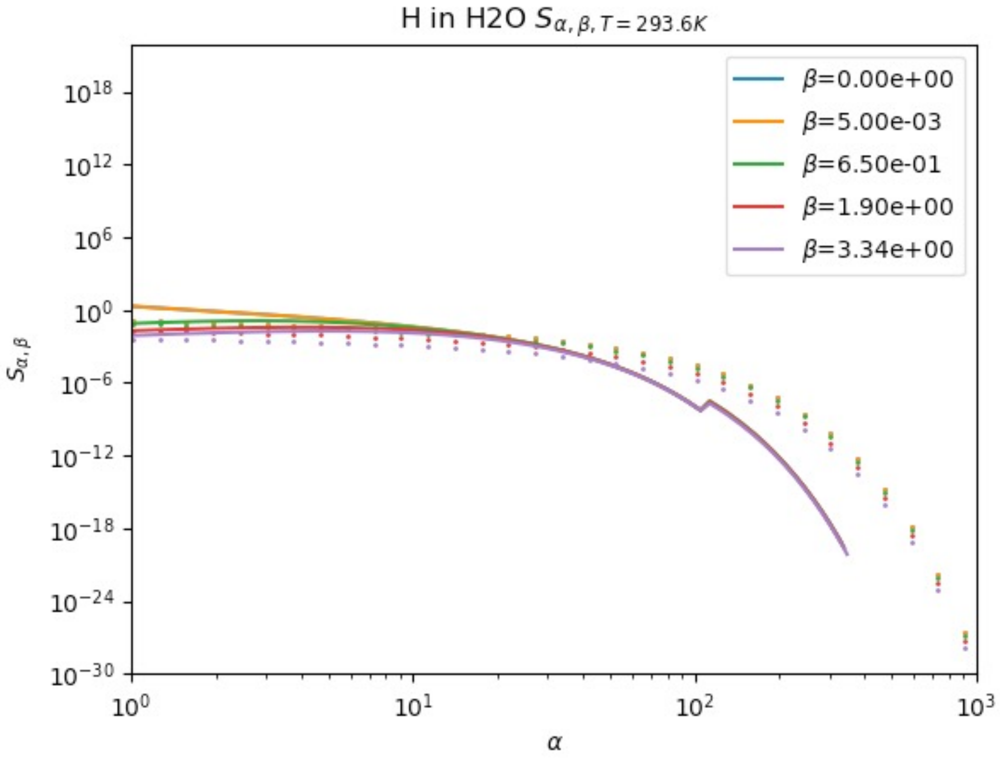
$$\beta = (E' - E)/kT$$

- A_0, M_n, σ_{bn}, $S_n(\alpha,\beta,T)$ are tabulated
- α,β grids in many evaluations aren't sufficient for spanning all (E, E', μ) of interest
  - Short collision time (SCT) approximation is appropriate for large α,β but generally not as α approaches 0
  - Extrapolation required for small α, but appears to be handled differently by processing codes
    - Especially relevant for forward scattering where E' ≈ E

Transition from tabulated S(α,β) to SCT is mostly smooth at the high-α end…

Solid lines = tabulated, dotted lines = SCT





- H in ZrH: S(α,β) tabulated from α = 0.504 up to α = 240
- H in H20: from α = 1.002e-5 up to α = 1581, but switches to SCT earlier for most values of β

… but SCT falls off too fast at the low end.

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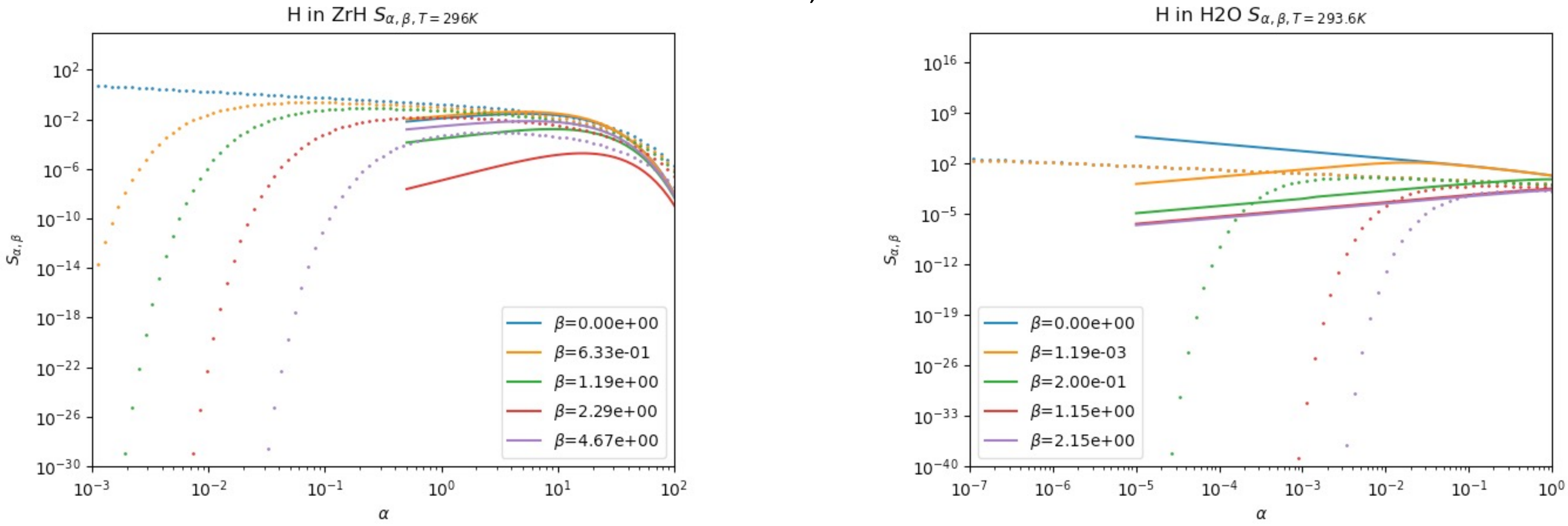

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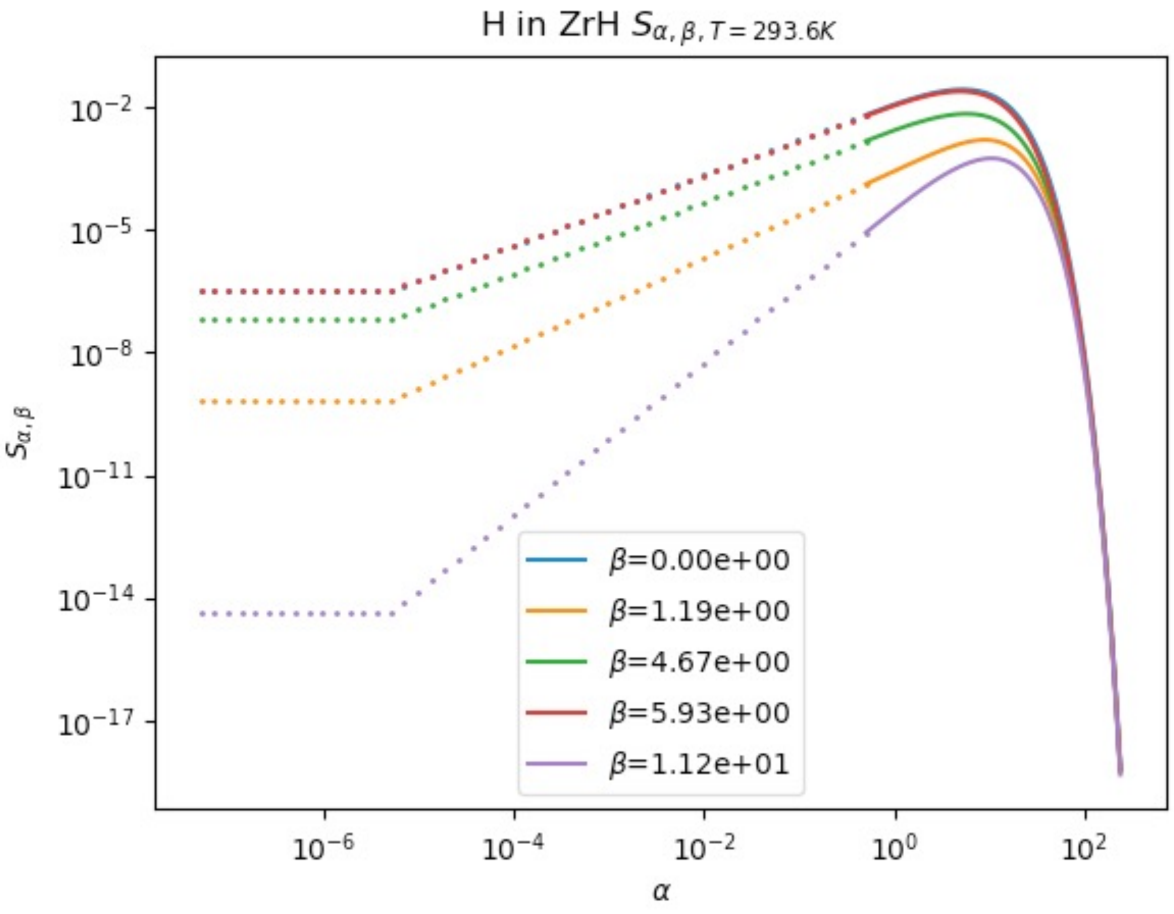
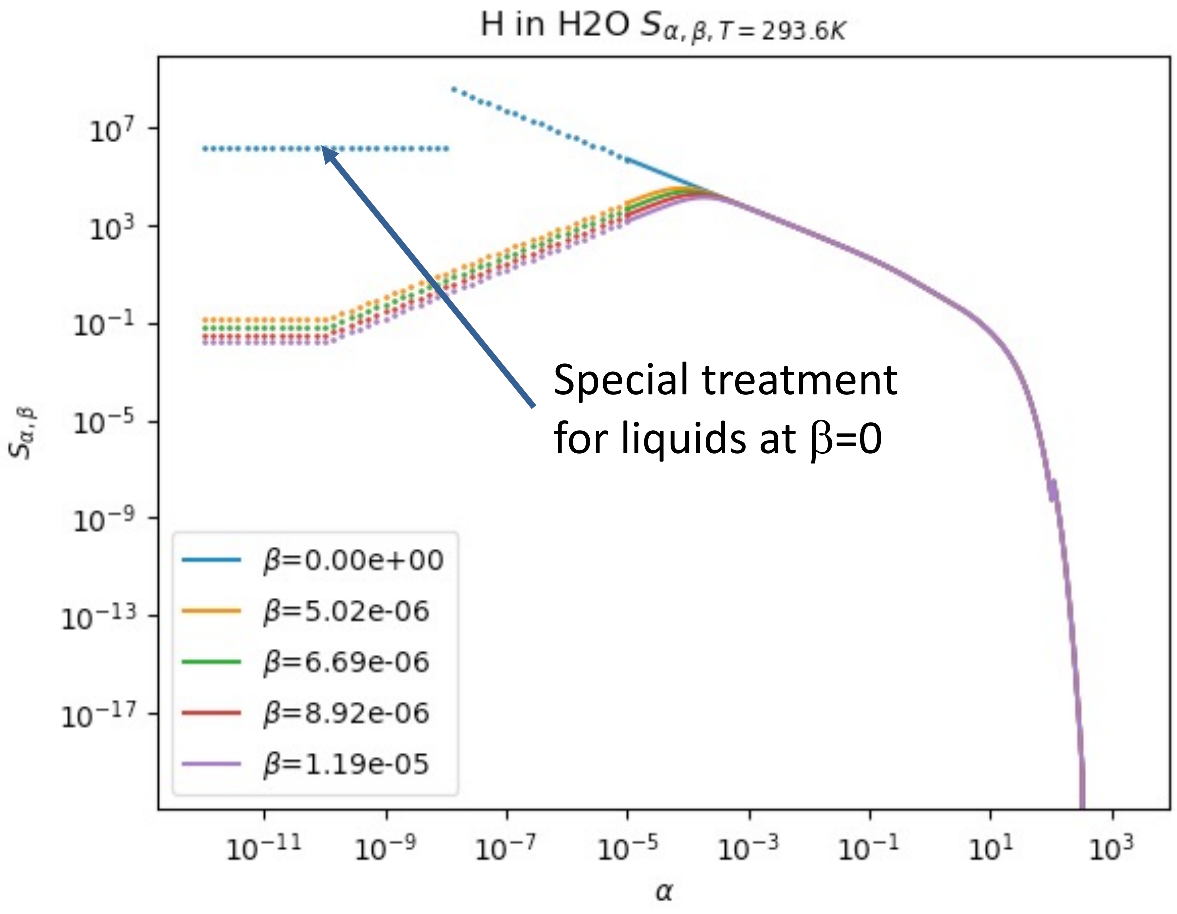
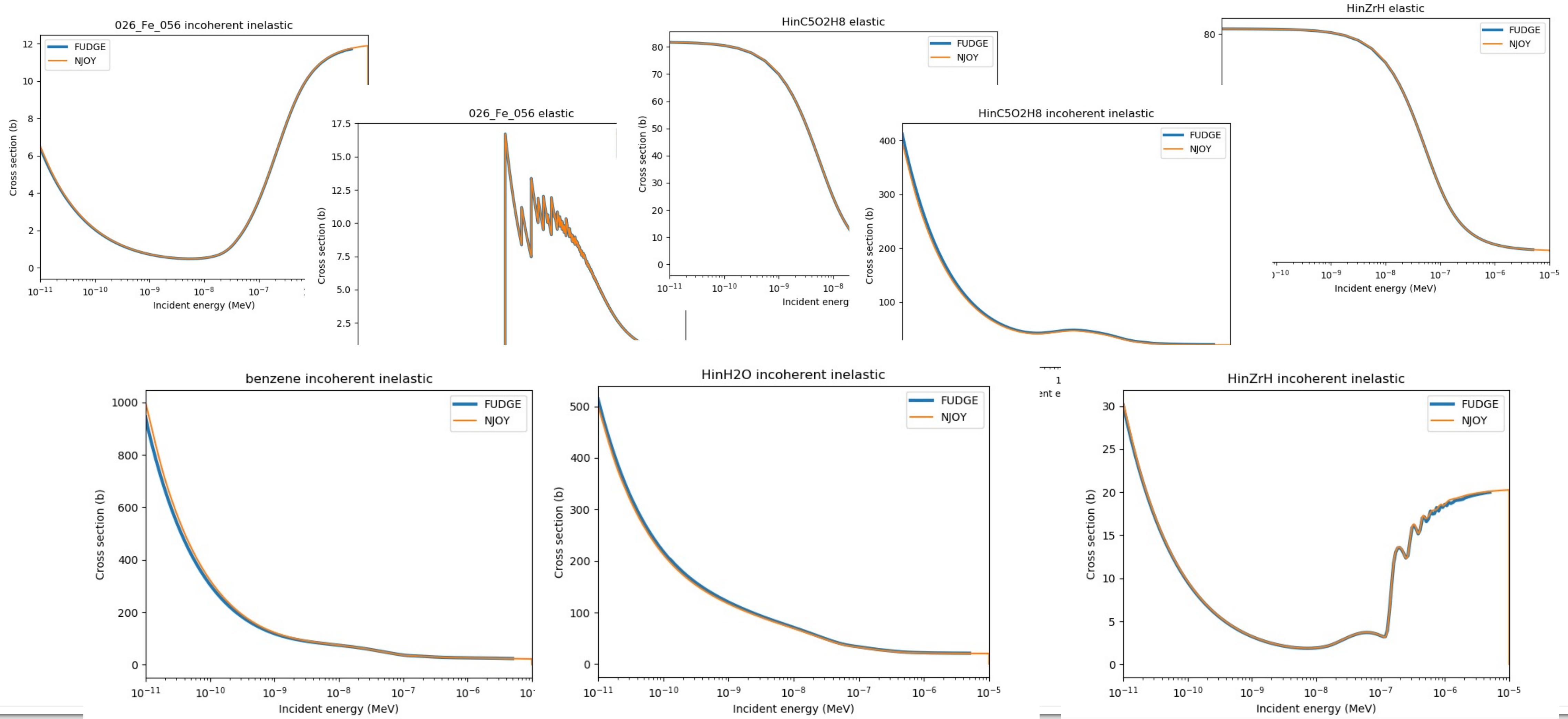
FUDGE uses power-law extrapolation for up to 5 orders of magnitude in α, then switches to S = constant

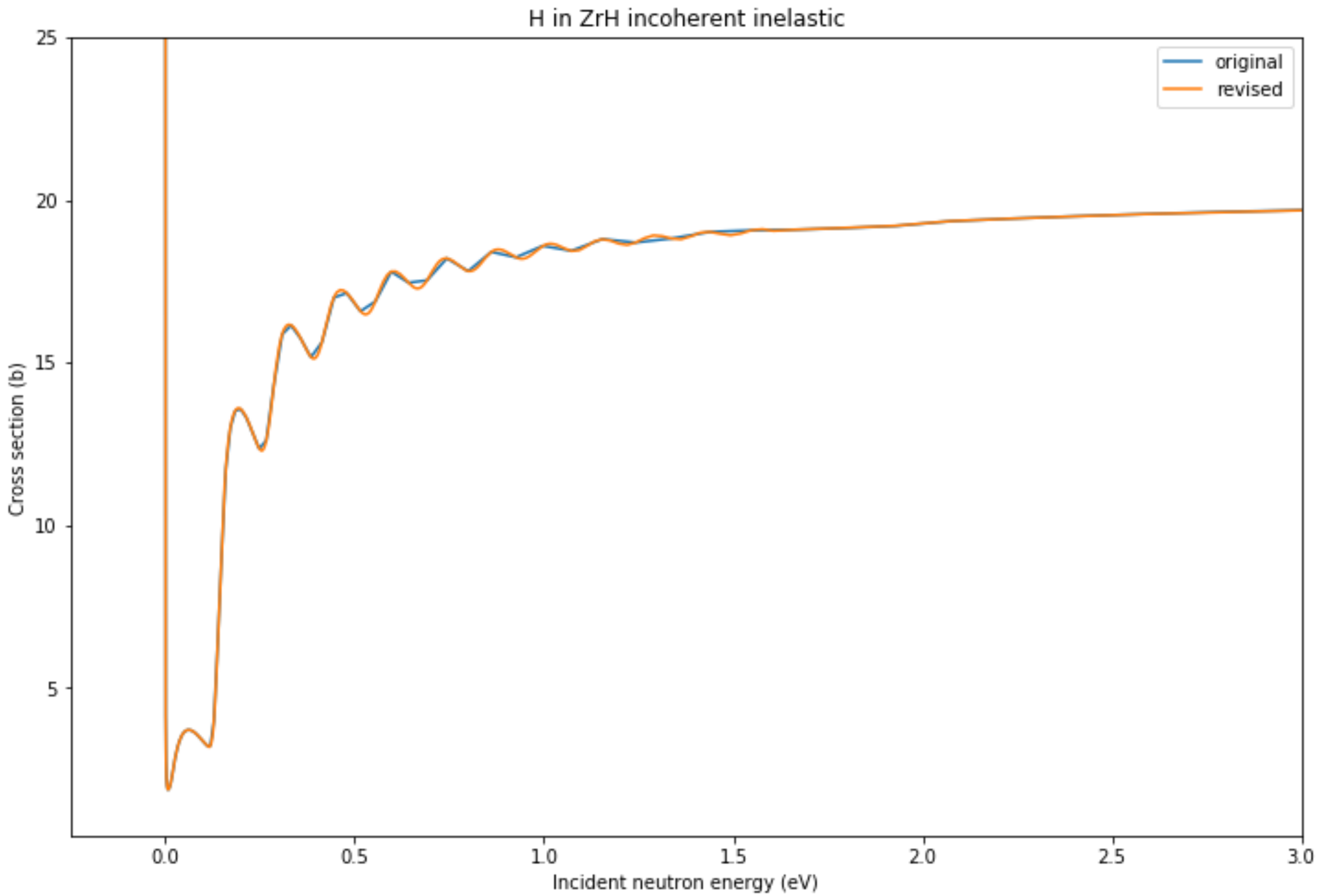




FUDGE TNSL cross sections compared to NJOY
Mostly agree, some differences at low incident energy…

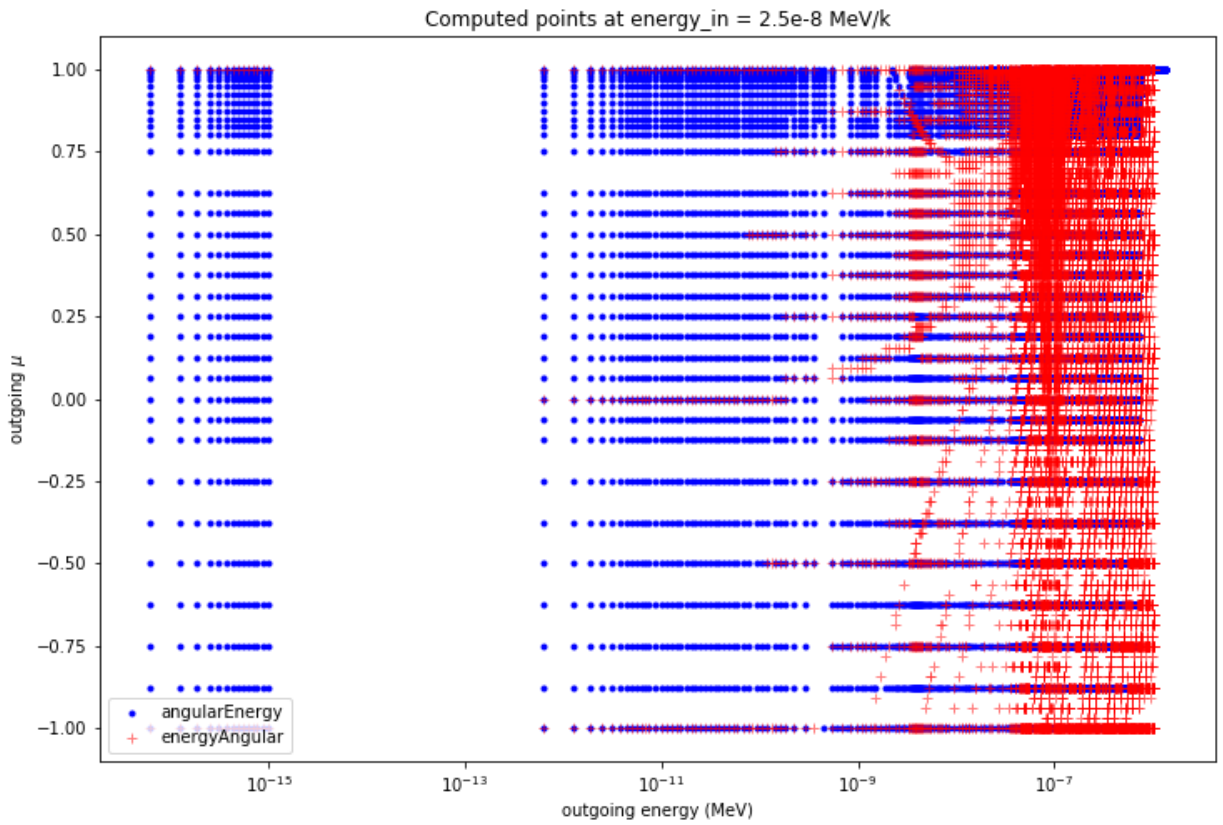


Recent update: iteratively add points to refine cross section



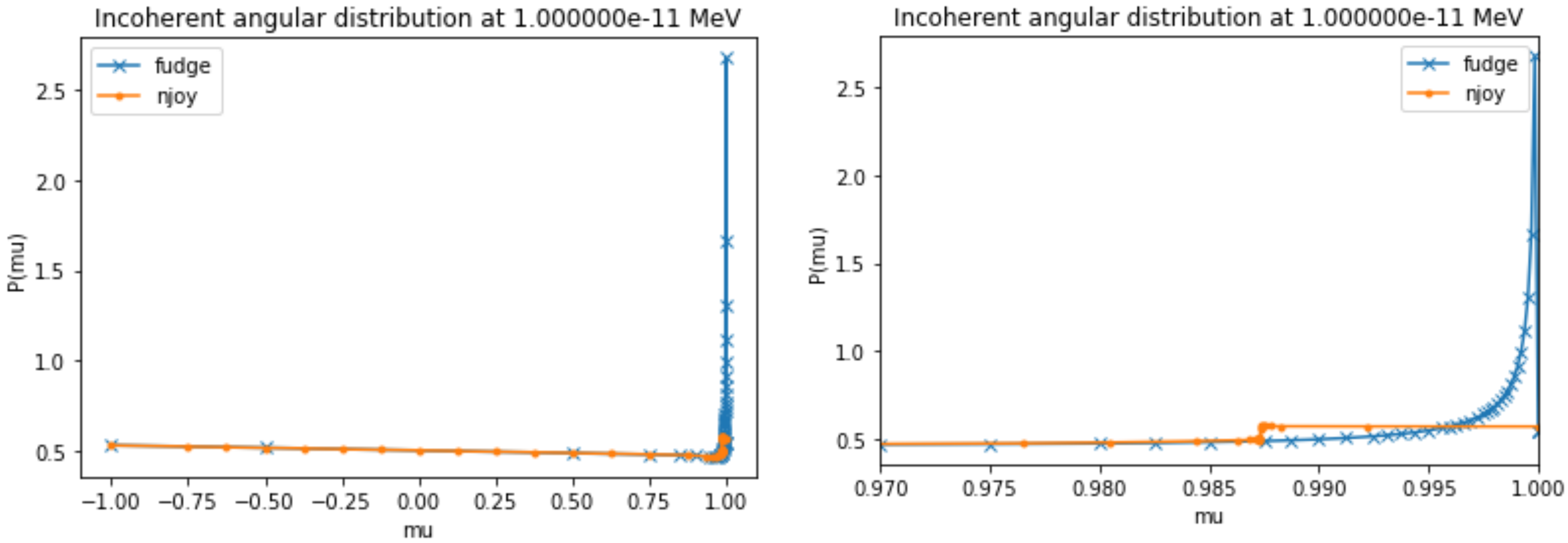
Recently switched incoherent inelastic distribution storage from P(E’|E,μ) to P(μ|E, E’)

- P(E’|E,μ) originally used for compatibility with legacy LLNL format ENDL, but storing a μ distribution for each incident / outgoing energy is more efficient



FUDGE / NJOY differences appear to originate with how each code handles extrapolation to small α

- Different approximations for forward scattering in H_2O near $E = E' = 10^{-11}$ MeV
  - Note: using THERMR with iform=1 option for easier comparison

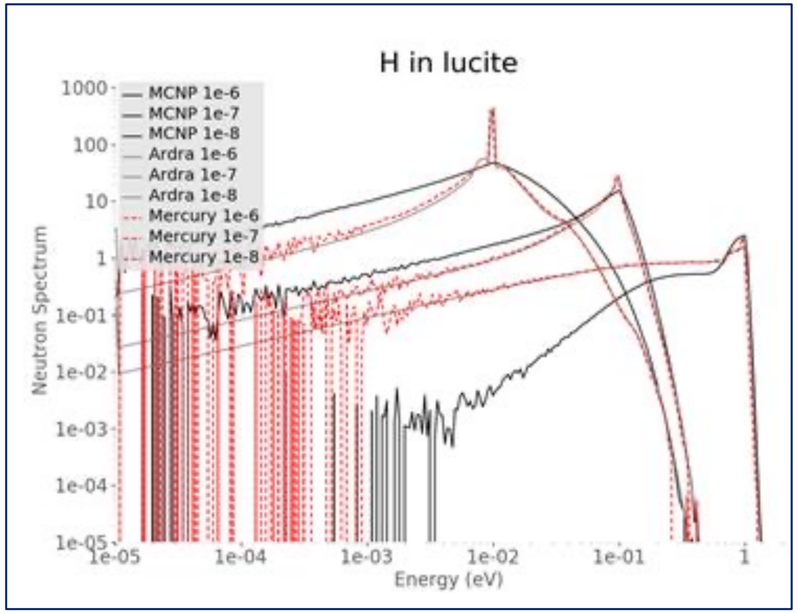


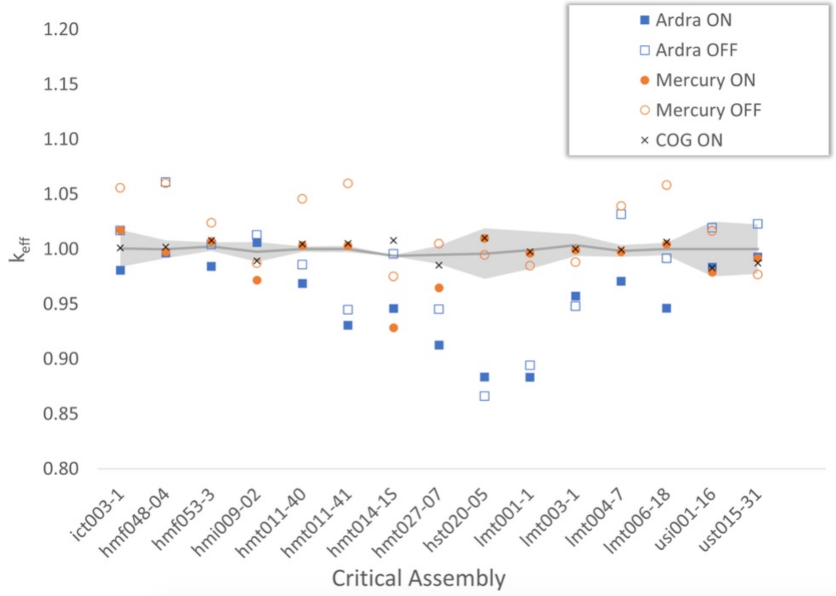
- Better would be to improve documentation on how extrapolation should be done

Additional TNSL testing: run broomsticks, critical assemblies and full-scale reactor problems

- Processed GNDS data used with Mercury (MC transport) and Ardra (deterministic)
  - Results compared against MCNP/ENDF80SaB2
  - Modeled critical assemblies, ACRR reactor in several configurations

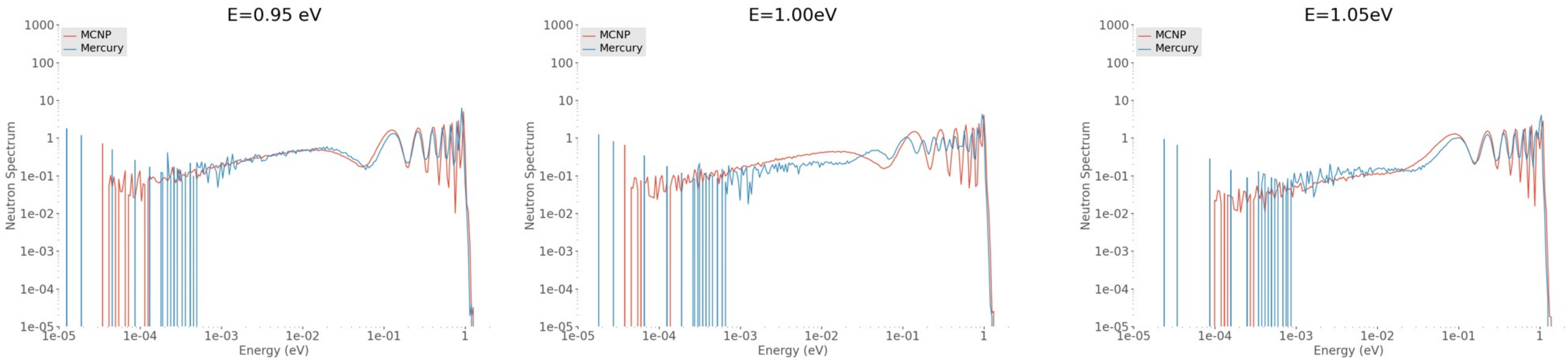
- Also exported to COG (via legacy ENDL format) for further testing by LLNL Criticality Safety group
  - Minor complication: ENDL requires P(μ | E) * P(E' | E, μ) while ACE requires P(E', μ | E)





MCNP and MCGIDI (Monte Carlo sampling library in GIDI+) handling interpolation differently

- To understand Mercury/MCNP broomstick differences, FUDGE was modified to process H in ZrH on the same incident energy grid as ENDF80SaB2 ACE files.
- Broomsticks then run with incident energies at grid points (0.95 and 1.05 eV) and at points between… results indicate an interpolation bug in MCGIDI



Conclusion:

- FUDGE TNSL processing capabilities are improving
  - New development focuses on reading and writing GNDS, but FUDGE also supports writing to ACE and ENDL
  - Work provides a chance to compare in-depth with other codes

- TNSL processing is mostly complete, but MCGIDI sampling has room for improvement
  - Revisit interpolation + improved strategies for sampling coherent / incoherent elastic